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SOME ADDITIONAL RESULTS ON PRINCIPAL COMPONENTS ANALYSIS OF THREE-MODE DATA BY MEANS OF ALTERNATING LEAST SQUARES ALGORITHMS

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Kroonenberg and de Leeuw (1980) have developed an alternating least-squares method TUCKALS-3 as a solution for Tucker's three-way principal components model. The present paper offers some additional features of their method. Starting from a reanalysis of Tucker's problem in terms of a rank-constrained regression problem, it is shown that the fitted sum of squares in TUCKALS-3 can be partitioned according to elements of each mode of the three-way data matrix. An upper bound to the total fitted sum of squares is derived. Finally, a special case of TUCKALS-3 is related to the Carroll/Harshman CANDECOMP/PARAFAC model.

Key words: partitioning of least-squares fit, rank-constrained regression, Candecomp, Parafac.

Introduction

Kroonenberg and de Leeuw (1980) have offered an alternating least-squares solution (TUCKALS-3) for the three-mode principal component model developed by Tucker (1963, 1964, 1966). Their solution is based on the observation that the optimal core matrix can be expressed uniquely and explicitly in terms of the data and the component matrices for the three modes. The latter component matrices are optimized by an alternating least-squares algorithm.

The present paper is aimed at offering some results for TUCKALS-3 in addition to those given by Kroonenberg and de Leeuw. First, it will be shown that the fitted sum of squares in TUCKALS-3 can be partitioned according to elements of each mode. This result is based on a rederivation of TUCKALS-3 in terms of a rank-constrained regression problem. Next, an upper bound to this fitted sum of squares will be derived. Finally, a relationship between a special case of TUCKALS-3 and the Carroll/Harshman CANDECOMP/PARAFAC model (see Harshman & Lundy, 1984a, 1984b and Carroll & Pruzansky, 1984) will be demonstrated.

In the next section the main features of TUCKALS-3, as given by Kroonenberg and de Leeuw (1980), will be revisited.

The Tucker-3 Model and the TUCKALS-3 Solution

Let Z be a three mode data matrix of order $\ell \times m \times n$ with elements z_{ijk}, $i = 1, \ldots, \ell$; $j = 1, \ldots, m$; $k = 1, \ldots, n$. The least-squares fitting of the Tucker-3 model implies

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minimizing the residual sum of squares

$$\sum_{i,j,k} (z_{ijk} - \hat{z}_{ijk})^2, \tag{1}$$

where $\hat{z}_{ijk}$ is a weighted sum of elements of an $\ell \times s$ matrix G, an $m \times t$ matrix H, an $n \times u$ matrix E, and an $s \times t \times u$ core matrix C (Kroonenberg & de Leeuw, 1980, p. 70). In TUCKALS-3 the matrices G, H and E are restricted to be column-wise orthonormal.

Let Z_ℓ be the $\ell \times mn$ matrix containing the m lateral $\ell \times n$ planes of Z, then the associated fitted parts of Z can be collected in the $\ell \times mn$ matrix

$$\hat{Z}_\ell = GC_s(H' \otimes E') \tag{2}$$

where C_s is the $s \times tu$ matrix containing the t lateral $s \times u$ planes of C, and $\otimes$ is the Kronecker product. Clearly, minimizing (1) is equivalent to minimizing

$$f(G, H, E, C) = \| Z_\ell - \hat{Z}_\ell \|^2 = \| Z_\ell - GC_s(H' \otimes E') \|^2. \tag{3}$$

For fixed G, H, and E the minimizing C_s is uniquely defined as

$$C_s = G'Z_\ell(H \otimes E) \tag{4}$$

(Penrose, 1956, p. 18). Hence minimizing (1) reduces to minimizing

$$g(G, H, E) = \| Z_\ell - GG'Z_\ell(HH' \otimes EE') \|^2, \tag{5}$$

which, in turn, is equivalent to maximizing

$$p(G, H, E) = \text{tr } G'Z_\ell(HH' \otimes EE')Z'_\ell G \stackrel{d}{=} \text{tr } G'PG. \tag{6}$$

In a completely parallel fashion, it can be shown that

$$p(G, H, E) = \text{tr } H'Z_m(EE' \otimes GG')Z'_m H \stackrel{d}{=} \text{tr } H'QH, \tag{7}$$

where Z_m is the $m \times \ell n$ matrix containing the n transposed frontal $\ell \times m$ planes of Z, and that

$$p(G, H, E) = \text{tr } E'Z_n(GG' \otimes HH')Z'_n E \stackrel{d}{=} \text{tr } E'RE, \tag{8}$$

where Z_n is the $n \times \ell m$ matrix containing the ℓ horizontal $n \times m$ planes of Z, (Kroonenberg & de Leeuw, 1980, p. 72).

The TUCKALS-3 solution consists of iteratively improving G for fixed H and E, H for fixed G and E, and E for fixed G and H, starting from Tucker's final solution for G, H and E (Tucker, 1966, p. 297). That is, initially G consists of the principal s eigenvectors of $Z_\ell Z'_\ell$; H consists of the principal t eigenvectors of $Z_m Z'_m$, and E consists of the principal u eigenvectors of $Z_n Z'_n$. The procedure terminates when a necessary condition for a maximum is satisfied, that is, when simultaneously G contains the s principal eigenvectors of P, H contains the t principal eigenvectors of Q, and E contains the u principal eigenvectors of R. We shall now rederive the TUCKALS-3 solution from a generalized perspective.

An Alternative Approach to the Least Squares Fitting of the Tucker-3 Model

Kroonenberg and de Leeuw (1980, p. 70) noted that it is merely a matter of convenience to have G, H and E constrained to be orthonormal column-wise. This point will now be elaborated in a generalized approach to the Tucker-3 model, in which the orthonormality constraints are omitted. The derivation to be given below applies equally to G,

H and E but we shall only consider G in full detail. The derivations for H and E are completely analogous.

Let H and E be fixed matrices of rank t and u, respectively, and let $F \stackrel{d}{=} H \otimes E$. Then the TUCKALS-3 problem can be reduced to the problem of minimizing

$$h(G, C_s) \stackrel{d}{=} \| Z'_\ell - FC'_s G' \|^2, \tag{9}$$

refer to (3). Although it is possible to express the minimizing G in terms of C_s and vice versa, we shall simply address the problem of finding the optimal product $C'_s G' \stackrel{d}{=} W$ and consider the function

$$h(W) = \| Z'_\ell - FW \|^2. \tag{10}$$

The solution to this problem depends critically on the relative sizes of s, ℓ, and tu. Because $\ell \geq s$ and because $s \leq tu$ (Tucker, 1966, p. 288) we only need to consider the case $\ell \geq tu \geq s$ and the case $tu \geq \ell \geq s$. In the former case, solving (10) as an ordinary unconstrained least squares problem yields the well-known minimizing solution $W = (F'F)^{-1}F'Z'_\ell$ which generally has rank $tu \geq s$, because W is of order $tu \times \ell$. If $tu > s$ then this W cannot possibly be expressed as $W = C'_s G'$ where G' has rank s. Therefore, the unconstrained least-squares solution is not generally valid as a solution for (10) in the case $\ell \geq tu \geq s$.

Conversely, if $tu \geq \ell \geq s$ then $(F'F)^{-1}F'Z'_\ell$ generally has rank $\ell \geq s$ which is again incompatible with having a W of rank s or lower. In order to find a generally valid minimizing solution for (10) we shall want to minimize (10) subject to the constraint that W have rank s or lower. This constraint guarantees that W can always be expressed as $C'_s G'$ with G' of rank s. Let r denote the rank of the optimal W, $r \leq s$.

In order to minimize (10) subject to its constraint, let W be expressed in terms of an r-dimensional basis A, orthonormal in the metric $(F'F)$. That is, let

$$W = AB \tag{11}$$

for some $tu \times r$ matrix A satisfying $(A'F'FA) = I_r$, and some $r \times \ell$ matrix B. This takes care of the constraint on W, and makes for a straightforward solution. Combining (10) and (11) shows that we are to minimize

$$h(A, B) = \| Z'_\ell - FAB \|^2. \tag{12}$$

For any A meeting the constraint the minimizing B can be uniquely expressed as the unconstrained least squares solution

$$B = (A'F'FA)^{-1}A'F'Z'_\ell = A'F'Z'_\ell. \tag{13}$$

Therefore, it remains to minimize

$$h(A) = \| Z'_\ell - FAA'F'Z'_\ell \|^2 = \text{tr } Z_\ell Z'_\ell - \text{tr } A'F'Z'_\ell Z_\ell FA, \tag{14}$$

or, equivalently, to maximize

$$h^*(A) = \text{tr } A'F'Z'_\ell Z_\ell FA. \tag{15}$$

Consider the singular value decomposition

$$(F'F)^{-1/2}F'Z'_\ell = U\Gamma V' \tag{16}$$

with $U'U = V'V = I$ and Γ diagonal, nonnegative, and ordered. Combining (15) and (16) yields

$$h^*(A) = \text{tr } A'(F'F)^{1/2}U\Gamma^2U'(F'F)^{1/2}A. \tag{17}$$

Since $(F'F)^{1/2}A$ is a column-wise orthonormal matrix of rank $r \leq s$, (17) is maximized if and only if $(F'F)^{1/2}A$ contains the first s columns of U, possibly rotated. Let U_s be the $tu \times s$ matrix containing the first s columns of U. Then (17) is maximized if and only if

$$A = (F'F)^{-1/2}U_s T \tag{18}$$

for some orthonormal $s \times s$ matrix T, and hence the maximizing B is

$$B = T'U_s'(F'F)^{-1/2}F'Z_l' = T'U_s'U\Gamma V' = T'\Gamma_s V_s', \tag{19}$$

where Γ_s is the upper left $s \times s$ submatrix of Γ, and V_s is the $\ell \times s$ matrix containing the first s columns of V. It follows that (9) is minimal for

$$C_s'G' = AB = (F'F)^{-1/2}U_s\Gamma_s V_s'. \tag{20}$$

This leaves us with an infinity of possibilities for determining C_s and G. For instance, we may take

$$C_s' = (F'F)^{-1/2}U_s \qquad \text{and} \qquad G' = \Gamma_s V_s', \tag{21}$$

which implies that C_s' is column-wise orthonormal in the metric $(F'F)$, or we may take

$$C_s' = (F'F)^{-1/2}U_s\Gamma_s \qquad \text{and} \qquad G' = V_s', \tag{22}$$

and so on.

Parallel expressions to (21) and (22) can be obtained for updating the pair (H, C) and the pair (E, C) by keeping G and E and G and H fixed, respectively. As a result, taking G, H, and E column-wise orthonormal does not constrain the function (3). In addition, if G, H and E are taken column-wise orthonormal, then so is $F = H \otimes E$. In that case, C_s in (22) reduces to a row-wise orthogonal matrix. Clearly, parallel expressions hold for the core matrix "flattened" in the other two directions, which means that after convergence of TUCKALS-3 with orthonormal G, H and E the core matrix C is "orthogonal in every direction." This property of "all-orthogonality" has first been noted by Weesie and van Houwelingen (1983, p. 7), who derived an alternative for TUCKALS-3 which can handle missing data.

In TUCKALS-3 only the matrices G, H and E are explicitly updated according to (22) with column-wise orthornormal F, and its parallel expressions. However, C is not updated until convergence. This can be explained by the fact that C can be expressed in terms of G, H and E, see (4). When G, H or E is updated, C is updated implicitly. Therefore, TUCKALS-3 can be interpreted as an iterative procedure of updating the pairs (G, C), (H, C) and (E, C), respectively.

The present rederivation of TUCKALS-3 provides us with certain explicit expressions which facilitate a further examination of the fit in TUCKALS-3. This will be elaborated below.

Partitioning the Fit in TUCKALS-3

Since $p(G, H, E)$ is the sum of squares of $\hat{Z}$ it can be interpreted as a measure of fit in TUCKALS-3. It can be shown that, as in ordinary linear regression analysis, the residual sum of squares and the fit add up to the total observed sum of squares. That is,

$$\| \hat{Z}_\ell \|^2 + \| Z_\ell - \hat{Z}_\ell \|^2 = \| Z_\ell \|^2. \tag{23}$$

Instead of proving (23) we shall prove a stronger result, based on a partitioning of the fit over separate elements of each of the three modes. Our argument strengthens and generalizes results of Harshman and Lundy (1984a, p. 198) on the interpretation of squared PARAFAC loadings as variances.

Proof. Let it be assumed that the pair (G, C) has been updated by (20), thus minimizing (9) for fixed H and E. Then the fitted part of Z'_ℓ is

$$\hat{Z}'_\ell = F(F'F)^{-1/2}U_s\Gamma_s V'_s. \tag{24}$$

Consider the i-th column of $\hat{Z}'_\ell$, which is the fitted part of Z associated with the i-th element of the ℓ-mode, $i = 1, \ldots, \ell$. Let this column be denoted by $\hat{Z}'_\ell e_i$, where e_i is the i-th column of the $\ell \times \ell$ identity matrix. Then we have from (24)

$$\hat{Z}'_\ell e_i = F(F'F)^{-1/2}U_s\Gamma_s V'_s e_i. \tag{25}$$

It will now be shown that the sum of squares of the i-th column of Z'_ℓ equals the sum of fitted and residual sum of squares. That is,

$$\| Z'_\ell e_i \|^2 = \| \hat{Z}'_\ell e_i \|^2 + \| Z'_\ell e_i - \hat{Z}'_\ell e_i \|^2, \tag{26}$$

or, equivalently,

$$e'_i Z_\ell \hat{Z}'_\ell e_i = e'_i \hat{Z}_\ell \hat{Z}'_\ell e_i. \tag{27}$$

It follows at once from (25) that the right-hand side of (27) equals $e'_i V_s \Gamma_s^2 V'_s e_i$. In addition, from (25) and (16) we have

$$e'_i Z_\ell \hat{Z}'_\ell e_i = e'_i Z_\ell F(F'F)^{-1/2}U_s\Gamma_s V'_s e_i = e'_i V\Gamma U'U_s\Gamma_s V'_s e_i = e'_i V_s \Gamma_s^2 V'_s e_i, \tag{28}$$

which completes the proof of (27). □

It follows that the fitted sum of squares can be partitioned over elements of the ℓ-mode, when the pair (G, C) has been updated according to (20). Parallel expressions can be derived for the m-mode and the n-mode. Hence after convergence of TUCKALS-3 the fitted sum of squares can be partitioned over the elements of each mode. Obviously, (23) is an implication of this result. It should be noted that the result does not require column-wise orthonormality of G, H, and E.

A property that does require G, H and E to be column-wise orthonormal is the equality

$$\| C \|^2 = \| C_s \|^2 = p(G, H, E), \tag{29}$$

which readily follows from (4) and (6). This property guarantees that squared elements of the core matrix can be interpreted as contributions to the fit, which parallels the interpretation of squared singular values as "portions of variance explained" in ordinary PCA. It should be noted that (29) merely requires C_s to be optimal given orthonormal G, H and E, see (4). The special two-mode case of this property is well-known from ordinary regression analysis. That is, for an orthonormal set of predictors the fit equals the sum of squared regression weights.

It should be noted that the overall fit partitioning (23) has been derived from the optimality of C only, for fixed but not necessarily optimal G, H and E. On the other hand, the element-wise fit partitioning (26) has been obtained from the joint optimality of C and G, C and H, and C and E. Specifically, (26) was derived from (20), see (24). The question arises whether or not (26), like (23), could have been obtained from the optimality of C

only. If only C is optimal then we have a minimum for a function of the form $f(X) = \| B - AXC \|$, for fixed A, B and C, in the notation of Penrose (1956, Corollary 1). It can be verified that the minimizing X generates a best least squares approximation $\hat{B} = AXC$ which is orthogonal to $(B - \hat{B})$, *when B and $(B - \hat{B})$ are strung out as vectors.* However, this does not imply that each column of $\hat{B}$ is orthogonal to the corresponding column of $(B - \hat{B})$ and, in fact, counterexamples to this proposition can be constructed. For this reason, we do have to assume joint optimality of C and G, C and H and C and E to justify the element-wise fit partitioning (26).

An Upper Bound to the Fitted Sum of Squares

Tucker's original solution for the Tucker-3 model consists of performing a separate s-, t-, and u-dimensional component analysis on $Z_\ell Z'_\ell$, $Z_m Z'_m$, and $Z_n Z'_n$, respectively. The sums of the largest s, t, or u eigenvalues of these matrices can be taken as three—possibly different—measures of fit in Tucker's method. In TUCKALS-3 there is only one measure of fit (see (6), (7) or (8), and the previous section). The following lemma specifies a relationship between Tucker's three measures of fit and the fit in TUCKALS-3.

Lemma 1. Let λ_{gh} denote the g-th eigenvalue of $Z_h Z'_h$, $h = \ell$, m or n, then

$$p(G, H, E) \leq \min \left(\sum_{p=1}^{s} \lambda_{p\ell}, \sum_{q=1}^{t} \lambda_{qm}, \sum_{r=1}^{u} \lambda_{rn} \right), \tag{30}$$

where G, H, and E are column-wise orthonormal matrices of order $\ell \times s$, $m \times t$, and $n \times u$, respectively.

Proof. Consider

$$p(G, H, E) = \text{tr } G'Z_\ell(HH' \otimes EE')Z'_\ell G, \tag{31}$$

as in (6). Since $(HH' \otimes EE')$ is symmetric and idempotent, it has singular values which are either unity or zero, hence it is a suborthonormal matrix (ten Berge, 1983, Lemma 2). In addition, G is a suborthonormal matrix of rank s. It follows at once from the $n = 3$ case of Theorem 2 of ten Berge (1983) that

$$p(G, H, E) \leq \text{tr } (\Lambda_{\ell s}^{1/2} \Lambda_{\ell s}^{1/2}) = \text{tr } \Lambda_{\ell s}, \tag{32}$$

where $\Lambda_{\ell s}^{1/2}$ is the diagonal matrix containing the first s singular values of Z_ℓ in the upper left diagonal places, and zeroes elsewhere. Clearly, the squared singular values of Z_ℓ are eigenvalues of $Z_\ell Z'_\ell$, hence

$$p(G, H, E) \leq \text{tr } \Lambda_{\ell s} = \sum_{p=1}^{s} \lambda_{p\ell}. \tag{33}$$

The remainder of the proof can be given in a parallel fashion, by expressing $p(G, H, E)$ in terms of Z_m and Z_n, respectively, see (7) and (8). This completes the proof of Lemma 1. □

It was pointed out by an anonymous reviewer and by J. C. van Houwelingen (personal communication) that Lemma 1 merely provides a formal proof for a result that is intuitively obvious. Consider the approximation of Z_ℓ, for example, where TUCKALS-3 provides the best least squares estimate $\hat{Z}_\ell$, which is constrained to satisfy (2). In the parallel unconstrained case the best fitting $\hat{Z}_\ell$ entails $\| \hat{Z}_\ell \|^2 = \text{tr } \Lambda_{\ell s}$ (Eckart & Young, 1936). It follows that tr $\Lambda_{\ell s}$ is an upper bound to $p(G, H, E)$ in TUCKALS-3.

Lemma 1 can serve as a guideline for improving the fit in TUCKALS-3. That is, if the two-mode fit is relatively low in one particular mode, one might increase the rank of the component matrix G, H or E for that very mode in TUCKALS-3, as suggested by Kroonenberg (1983, p. 95).

A Relationship Between TUCKALS-3 and CANDECOMP/PARAFAC

There has been much discussion in the recent literature of the relationship between the TUCKALS-3 model and the CANDECOMP/PARAFAC model of Carroll and Harshman (compare Kroonenberg, 1983, chap. 3; and Harshman & Lundy, 1984a, pp. 169–178). One of the reasons for studying this relationship is that it may provide insights into the type of solution CANDECOMP/PARAFAC obtains, when it is applied to data that satisfy the TUCKER-3 model (Harshman & Lundy, 1984b, pp. 271–280). Another reason is that in some special cases the relationship between the two models is rather simple.

Consider the case where the third mode in TUCKALS-3 has only one component ($u = 1$) and the first two modes have the same number of components ($s = t$). Then the core matrix contains only one frontal $s \times s$ plane $C_1 = C$. There are some simple theoretical results in this case on the relationship between the TUCKALS-3 and the CANDECOMP/PARAFAC model due to de Leeuw (compare Kroonenberg, 1983, pp. 57–60). Here we show that if $u = 1$ and $s = t$, and TUCKALS-3 has converged to a global minimum of (1), then C is a diagonal matrix. It follows that in this case the TUCKALS-3 program computes a PARAFAC solution.

Let it be assumed that TUCKALS-3 has converged to a global minimum. From (4) we have

$$C_s = G'Z_\ell(H \otimes E), \tag{34}$$

for certain column-wise orthonormal G, H and E. Consider the $tu \times tu$ permutation matrix Π_1, which transforms C_s into an $s \times tu$ matrix $C_* = C_s\Pi_1$, containing the u frontal $s \times t$ planes of C. Also, consider the $mn \times mn$ permutation matrix Π_2, which transforms Z_ℓ into an $\ell \times mn$ matrix $Z_* = Z_\ell \Pi_2$, containing the n frontal $\ell \times m$ planes of Z. It can be verified that

$$\Pi_2'(H \otimes E)\Pi_1 = (E \otimes H). \tag{35}$$

Hence we have

$$C_* = C_s \Pi_1 = G'Z_\ell \Pi_2 \Pi_2'(H \otimes E)\Pi_1 = G'Z_*(E \otimes H) \tag{36}$$

as parallel expression to (34) in terms of frontal planes of C and Z.

Consider the special case of TUCKALS-3 with $s = t$ and $u = 1$. Then C contains only one frontal plane $C = C_*$ and we have

$$C = G'Z_*(E \otimes H) = G'\left(\sum_{k=1}^{n} e_k Z_k\right)H, \tag{37}$$

where Z_k is the k-th frontal plane of Z and e_k is the k-th element of the $n \times 1$ vector E, $k = 1, \ldots, n$. Consider the singular value decomposition

$$\left(\sum_{k=1}^{n} e_k Z_k\right) = MDN', \tag{38}$$

with $M'M = N'N = \mathrm{I}_m$ and D diagonal, ordered, and nonnegative. Then we have, after convergence of TUCKALS-3,

$$C = G'MDN'H, \tag{39}$$

and the TUCKALS-fit equals

$$\text{tr } CC' = \text{tr } G'MDN'HH'NDM'G = \text{tr } M'GG'MDN'HH'ND, \tag{40}$$

see (4), (6), and (39). The maximizing G and H satisfy the inequality

$$\text{tr } (M'GG'M)D(N'HH'N)D \leq \sum_{p=1}^{s} d_{pp}^2, \tag{41}$$

because $(M'GG'M)$ and $(N'HH'N)$ are suborthonormal and have rank s at the most (ten Berge, 1983, Lemma 4, Theorem 2). Let it be assumed that the s largest elements of D are distinct. Then it can be shown that (41) holds as an equality if and only if

$$M'GG'M = N'HH'N = \begin{pmatrix} I_s & 0 \\ 0 & 0 \end{pmatrix}. \tag{42}$$

Because G and H are globally optimal, they must satisfy (42). From (42) it follows that

$$M'G = \begin{pmatrix} T_1 \\ 0 \end{pmatrix} \quad \text{and} \quad N'H = \begin{pmatrix} T_2 \\ 0 \end{pmatrix} \tag{43}$$

for certain orthonormal $s \times s$ matrices T_1 and T_2. Therefore, we have

$$C = T_1' D_s T_2, \tag{44}$$

where D_s is the upper left $s \times s$ submatrix of D. From the all-orthogonality of C it follows that $T_1' D_s^2 T_1$ and $T_2' D_s^2 T_2$ are diagonal matrices. This implies that both T_1 and T_2 are diagonal and hence C is a diagonal matrix.

From the diagonality of C it follows that the fitted part of the k-th frontal plane of Z can be expressed as

$$\hat{Z}_k = GCe_k H' = GC_k H', \tag{45}$$

where $C_k \stackrel{d}{=} e_k C$, $k = 1, \ldots, n$. As a result, this special case of TUCKALS-3 can be interpreted as a CANDECOMP/PARAFAC model, with the additional constraint that G and H be column-wise orthonormal, and that the C_k be proportional (Harshman, 1970).

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